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THE CP-FTMW SPECTRUM OF 1-CHLOROMETHYL-1-FLUOROSILACYCLOPENTANE

TIARA PULLIAM, *Chemistry, Missouri University of Science and Technology, Rolla, MO, USA*; FRANK E MARSHALL, *Department of Chemistry, Missouri University of Science and Technology, Rolla, MO, USA*; THOMAS M. C. McFADDEN, GAMIL A GUIRGIS, *Department of Chemistry and Biochemistry, College of Charleston, Charleston, SC, USA*; G. S. GRUBBS II, *Department of Chemistry, Missouri University of Science and Technology, Rolla, MO, USA*.

Following a series of previously studied silicon-containing ring molecules, the rotational spectra of 1-chloromethyl-1-fluorosilacyclopentane were observed on a CP-FTMW spectrometer in the 6-18 GHz region. Using quantum chemical computational approaches, the molecule has multiple predicted stable conformers with both trans and gauche positions of the chlorine/fluorine pair with the gauche typically being largest in dipole, but the trans being lowest in energy. This presentation will discuss the observed conformers in the spectra and attempt to make predictions on which conformers are the most stable using spectral intensity arguments and comparisons to the quantum chemical calculations. Furthermore, the structure of this molecule will be compared to the previous silicon-containing ring molecules made by this group as well as others.